

WHAT IS CLAIMED IS:

1. A method for creating a database (5) which makes it possible in particular to select at least one catalyst suitable for a reaction, this method comprising the following stages:

a) preparing a plurality of different reaction media comprising the same reactivity probe and each comprising at least one catalyst,

b) analyzing, by an analytical method, each reaction medium after reaction,

c) assigning a result of the analysis according to stage b) to the reactivity probe in the database, this result characterizing the different reaction products obtained from this reactivity probe, the database being a relational database comprising a first entity (5a) in which is recorded information relating to the reaction units listed in the base, a second entity (5b) comprising information relating to the state of the bonds of at least one reaction unit listed in the first entity, a third entity (5c) in which is recorded information associated with the different reaction media and at least one fourth entity (5d) in which is recorded information related to the analytical results of the reaction media on conclusion of a reaction.

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2. A method for creating a database (5) which makes it possible in particular to select at least one catalyst suitable for a reaction, this method comprising the following stages:

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a) preparing a plurality of different reaction media comprising the same reactivity probe and each comprising at least one catalyst,

b) analyzing, by an analytical method, each reaction medium after reaction,

5 c) assigning a result of the analysis according to stage b) to the reactivity probe in the database, this result characterizing the different reaction products obtained from this reactivity probe,  
reaction units being listed individually in the  
10 database, the units being present on the reactivity probes, and  
for at least a portion of the reaction units listed, information is associated with each unit listed, in particular on the states of the bonds, targeted at  
15 describing the degree of reactivity of the bonds which are associated with it.

3. A method for creating a database (5) which makes it possible in particular to select at least one  
20 catalyst suitable for a reaction, this method comprising the following stages:

a) preparing a plurality of different reaction media comprising the same reactivity probe and each  
25 comprising at least one catalyst,

b) analyzing, by an analytical method, each reaction medium after reaction, the result of the analysis characterizing different reaction products obtained  
30 from this reactivity probe,

c) assigning a result of the analysis according to stage b) to the reactivity probe in the database, reaction units being listed individually in the  
35 database, the units being present on reactivity probes, the database comprising information which informs about the influence of the structural environment of a listed reaction unit on its reactivity.

4. The method as claimed in one of the preceding  
claims, characterized in that the plurality of  
different reaction media comprises at least two  
5 reaction media comprising different catalysts.

5. The method as claimed in any one of the preceding  
claims, characterized in that the analytical method is  
a liquid or gas chromatography method.

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6. The method as claimed in any one of the preceding  
claims, characterized in that stages a) to c) are  
repeated for a plurality of different reactivity probes  
and/or a plurality of different reaction media.

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7. The method as claimed in any one of the preceding  
claims, characterized in that, for one reactivity probe  
at least, a file is generated collating the group of  
the results covering all the conversions which have  
20 been carried out on said probe.

8. The method as claimed in any one of the preceding  
claims, characterized in that the reactivity probe  
comprises at least one reaction unit, preferably at  
25 least two reaction units.

9. The method as claimed in any one of the preceding  
claims, characterized in that the reaction media are  
chosen in order to carry out at least one of the  
30 following reactions: reactions for the formation or  
breaking of bonds, in particular C-C; -CO; -CN; C=N;  
C=C bonds.

10. A method for selecting at least one catalyst of  
35 use in the chemical conversion of at least one reaction  
unit, characterized in that it comprises at least the  
stages consisting in:

x) acquiring data relating to said conversion and, if appropriate, to the structural environment of the reaction unit to be converted,

5 y) identifying, in a database informing about the reactivity of a group of catalysts with regard to reaction units listed in the database and present on reactivity probes, at least one listed reaction unit related to the unit to be converted,

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z) selecting, in the database, according to the listed reaction unit thus identified, on the one hand, and the conversion to be carried out, on the other hand, at least one catalyst having the reactivity  
15 required for the conversion.

11. The method as claimed in the preceding claim, characterized in that said database was created according to a method as disclosed in any one of claims  
20 1 to 9.

12. The method as claimed in either one of claims 10 and 11, characterized in that the conversion takes place during a chemical reaction chosen from  
25 halogenation, reduction, hydrogenation, oxidation, hydrolysis, dehydration or esterification reactions, acidic or basic catalytic reactions, metallocatalyzed multicomponent reactions, trimerization reactions, reactions for the formation of heterocycles, pericyclic  
30 reactions or thermal and/or photochemical reactions.

13. The method as claimed in any one of claims 10 to 12, characterized in that the conversion is chosen from: reduction of imine to give amine, cleavage of a  
35 benzyl C-N or C-O bond, reduction of a halide, reduction of a nitro functional group to give amine or of a nitrile to give amine, reduction of amide, reduction of an alkyne unit, reduction of a ketone to

give alcohol, reduction of a ketone to give alkane and cleavage of an ether unit.

14. The method as claimed in any one of claims 10 to 5 13, characterized in that the acquisition of the data in stage a) comprises the formulation of a request mentioning the reaction unit concerned and the nature of the conversion to which it is desired to subject it.

10 15. The method as claimed in any one of claims 10 to 14, characterized in that the conversion is formulated by indicating the variation in the state of the bonds of the functional groups to be converted or to be retained in each reaction unit resulting from the 15 conversion or the difference in the state of the bonds in the reaction unit under consideration between the states before and after conversion.

16. The method as claimed in any one of claims 10 to 20 15, characterized in that the acquisition of data comprises the formulation of a request relating to the conversion and/or the nonconversion of at least two different reaction units.

25 17. The method as claimed in any one of claims 10 to 16, characterized in that, in the case of a first reaction unit to be converted and of a second reaction unit not to be converted, this first reaction unit and this second reaction unit being present on a starting 30 compound, the request is targeted at selecting a catalyst capable of carrying out the conversion of the first unit with a satisfactory yield while leaving the second intact or at the very least converting it to a sufficiently insignificant extent.

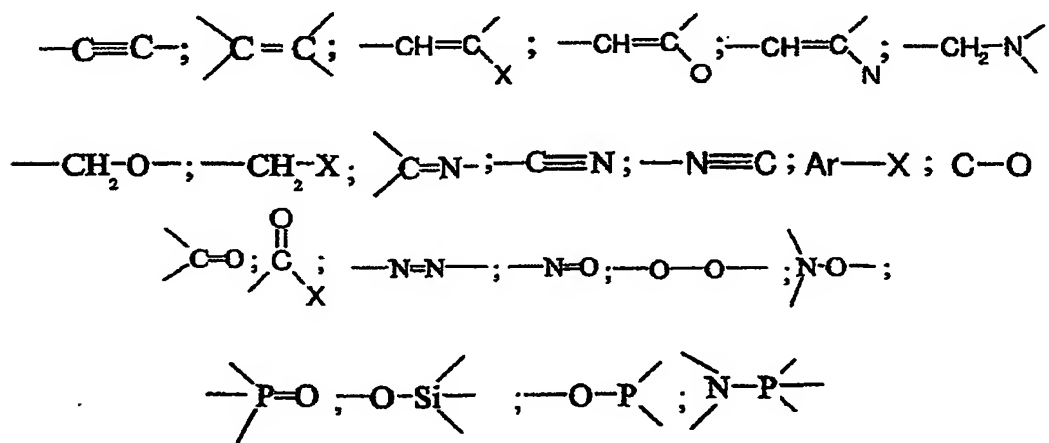
35 18. The method as claimed in any one of claims 10 to 17, characterized in that the acquisition of data in stage a) is carried out by formulating a request for

the conversion of at least one starting compound, the method comprising the analysis of the starting and final compounds for the purpose of identifying the reaction unit or units which react and that or those  
5 which do not react.

19. The method as claimed in any one of claims 10 to 18, characterized in that it comprises:

- 10 - the breakdown into different substructures of a starting compound involved in a reaction,
- the identification of the reaction unit or units to be converted and, if appropriate,
- 15 - the identification of the reaction unit or units which have to be retained.

20. The method as claimed in any one of the preceding claims, claim 1, characterized in that the reaction unit is chosen from:



with X representing a halogen atom.

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21. The method as claimed in any one of the preceding claims, characterized in that the database comprises, for each catalyst listed, information relating to the

reaction medium in which it was tested for its catalytic activity.

22. The method as claimed in any one of the preceding  
5 claims except claim 2, characterized in that, for at  
least a portion of the reaction units listed in the  
database, information is associated with each unit  
listed targeted as describing the state of the bonds  
which are associated with it.

10 23. The method as claimed in either one of claims 2  
and 22, characterized in that the state of the bonds is  
an integer ranging from 0 to 3.

15 24. The method as claimed in any one of the preceding  
claims except claim 4, characterized in that the  
database comprises information which informs about the  
influence of the structural environment of a listed  
reaction unit.

20 25. The method as claimed in any one of the preceding  
claims, characterized in that the database comprises  
data which inform about the activity of a portion at  
least of the catalysts listed according to different  
25 reaction conditions, in particular the temperature of  
the reaction medium, the acidity, the pressure, the  
presence of solvents or the analytical method.

30 26. A method for providing at least one catalyst which  
can be used to convert at least one reaction unit of at  
least one compound according to a given chemical  
reaction, characterized in that it comprises, in  
addition to stages x), y) and z) defined in claim 10,  
at least one stage of providing the catalyst or  
35 catalysts thus selected, and in particular the  
manufacture of said catalyst.

27. A method for creating a database (5) which makes it possible in particular to select at least one catalyst suitable for a reaction, this method comprising the following stages:

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a) preparing a plurality of different reaction media comprising the same reactivity probe and each comprising at least one catalyst,

10 b) analyzing, by an analytical method, each reaction medium after reaction,

c) assigning a result of the analysis according to stage b) to the reactivity probe in the database, this  
15 result characterizing the various reaction products obtained from this reactivity probe.